Machine Learning Flavour Tagging for Future Higgs Factories

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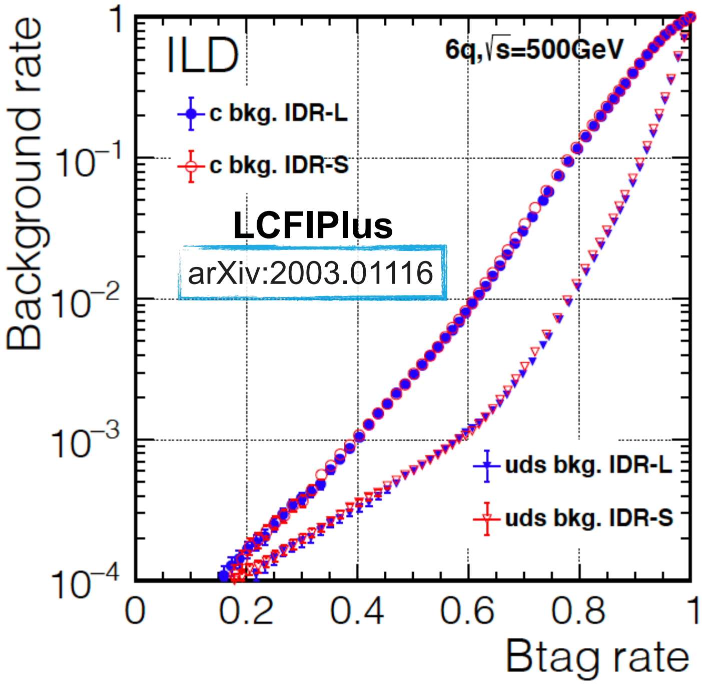
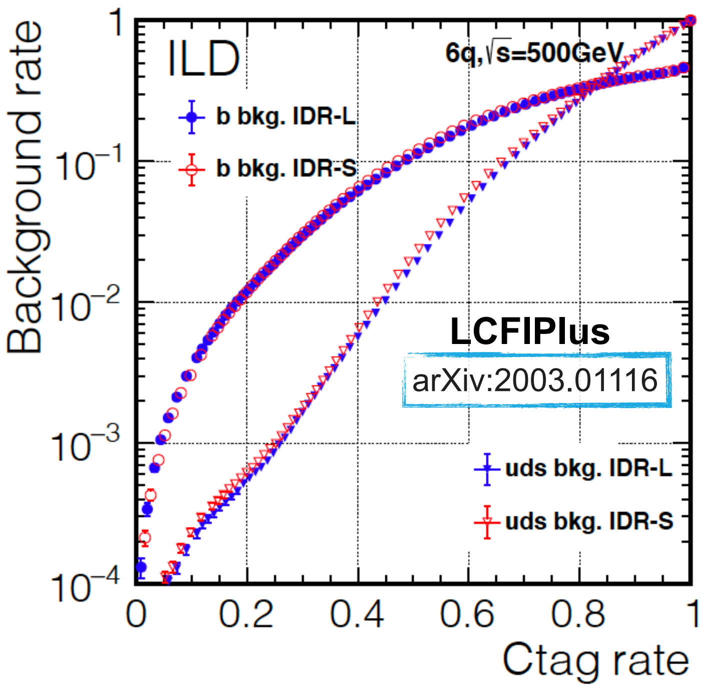
HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

Introduction

- **current standard** for heavy flavour tagging at ILD: **LCFIPlus**
- based on TMVA (BDTs)

arXiv:1506.08371,
https://github.com/lcfiplus/LCFIPlus

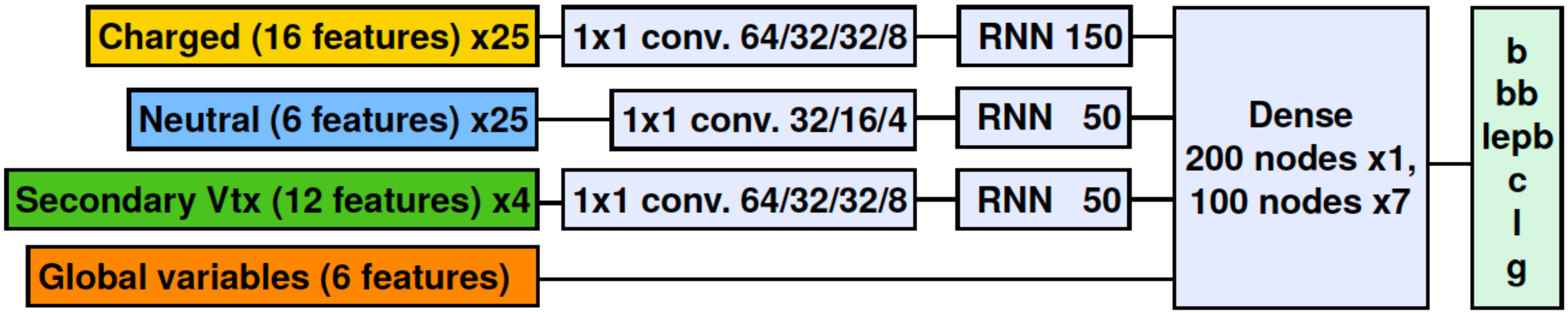




➡ Can the **heavy flavour tagging** be **improved** by replacing the BDTs used in LCFIPlus **with (deep) NNs**?

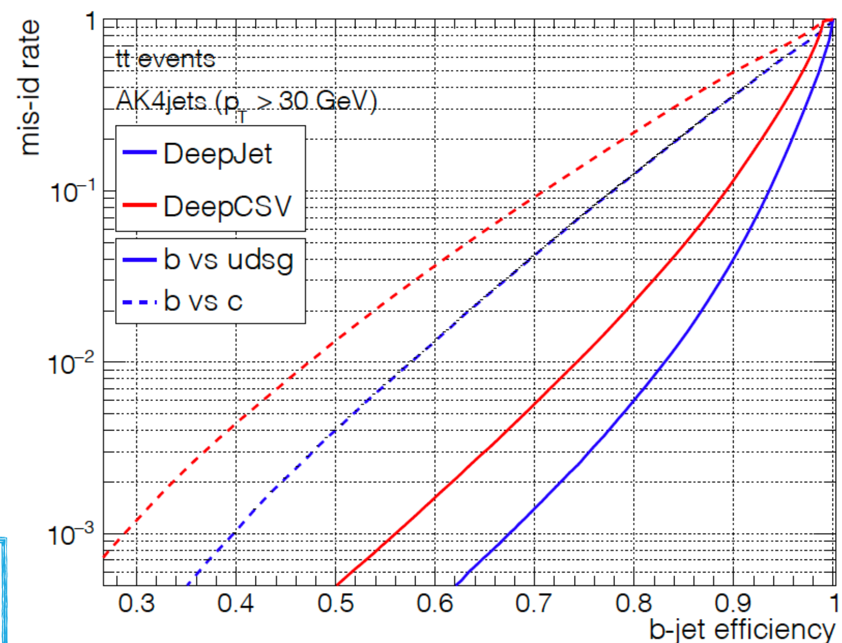
this work: **application of CMS DeepJet and ParticleNet to ILD**

CMS DeepJet

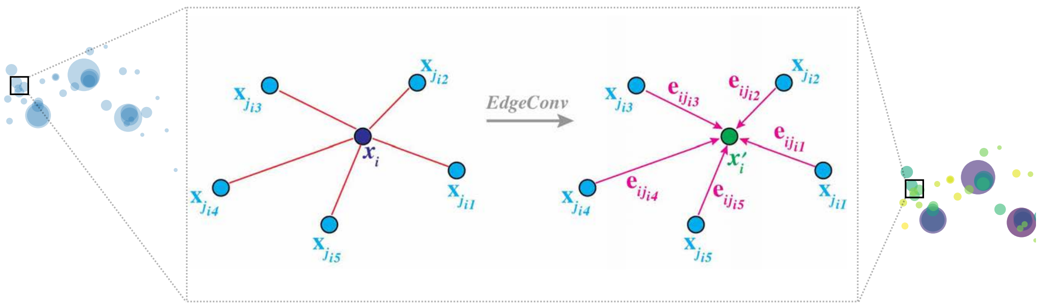


- successfully applied in many CMS analyses
- allows for **usage of low-level features** from **many jet constituents**
- able to deal with **variable length of inputs**
- allows for **ordering** of particles **according to** their assumed **importance**
- **large gain in performance** compared e.g. to FCNN (DeepCSV)

Jet Flavour Classification Using DeepJet arXiv:2008.10519,
Identification of heavy-flavour jets with the CMS detector in pp collisions at 13 TeV arXiv:1712.07158



ParticleNet



arXiv:1902.08570, *Pushing the Limit of Jet Tagging With Graph Neural Networks*, Huilin Qu, talk at ML4Jets2021, July 7, 2021

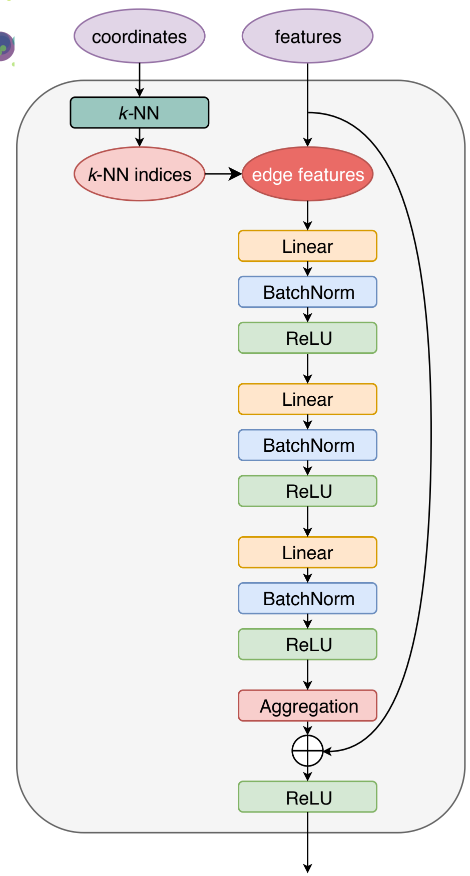
- treat jet as „particle cloud“
- input: **jet constituents**

key building block: **edge convolution**

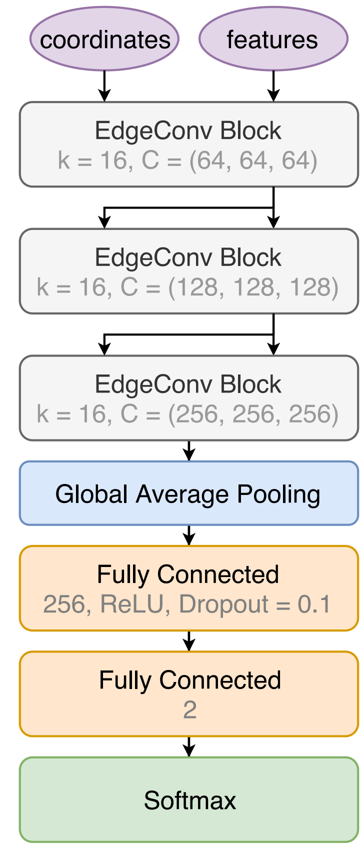
- particle cloud: graph, each point: vertex, connections between each point & k nearest neighboring points: edges
- learn an „**edge feature**“ for each pair:

$$e_{ij} = \mathrm{MLP}(x_i, x_j)$$

- **MLP**: parameters **shared among all edges**
- **aggregation** of edge features: $x_i' = \mathrm{mean}_j\, e_{ij}$



edge convolution



ParticleNet

Training data & data pre-processing

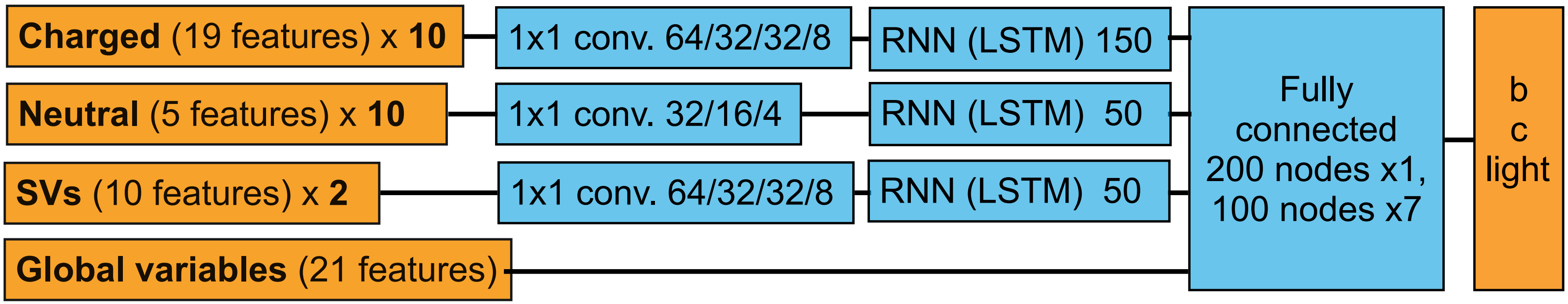
- study **events with 6 jets** (b,c,u,d,s)
  - 1 : 1 : 3 for b : c : light
- run PV & SV finder, jet clustering and vertex refinement of LCFIPlus
- **split sample** into training, validation and test (75% / 12.5% / 12.5%)
- **training data**: oversampling of b & c jets performed to get same number of b,c & light jets
  - ➡ ~4.3 Mio. jets in total
- **validation data**: keep orginial composition (1 : 1 : 3 for b : c : light)
  - ➡ ~394.000 jets in total

data pre-processing:

- if a value of a features is not available, the value is set to -10
- **normalize input features** to mean 0, std 1

DeepJet

DeepJet: architecture



- classify jets into **three classes**: b jets, c jets & light jets
- **ordering of input particles** by (as applied in CMS)
  - impact parameter significance for charged jet constituents
  - shortest angular distance to a secondary vertex (by momentum if there is no secondary vertex) for neutral jet constituents
  - flight distance significance for secondary vertices

DeepJet: input features

global variables

p^{jet}, p_T^{jet},

$N_{charged\ jet\ const.}$, $N_{neutral\ jet\ const.}$, N_{SV}

additional global variables from LCFIPlus

21 input features

charged jet constituents

p^{track}/p^{jet}, p_T^{track} (rel. jet), $\vec{p}^{\,track} \cdot \vec{p}^{\,jet}/p^{jet}$

ΔR(track, jet)

impact parameter & significances

track reconstructed in PV?

lepton related variables

pid variables

$\chi 2$/ndf

19 input features

neutral jet constituents

$p^{neutral\ const.}$, $p^{neutral\ const.}/p^{jet}$

ΔR(jet, neutral const.)

is photon?

$E_{HCAL}/E_{HCAL+ECAL}$

5 input features

secondary vertices

m_{SV}

$N_{tracks\ in\ SV}$

ΔR(SV, jet)

E_{SV}/E_{jet}, E_{SV}

cos(flight direction$_{SV}$, $\vec{p}_{SV}$)

3D IP and significance

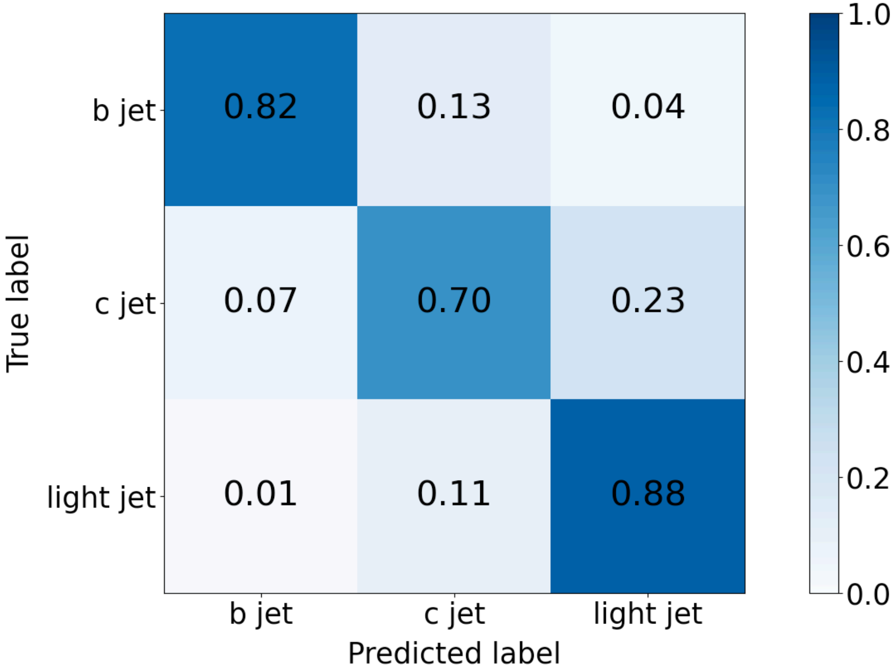
$\chi 2$, ndf

10 input features

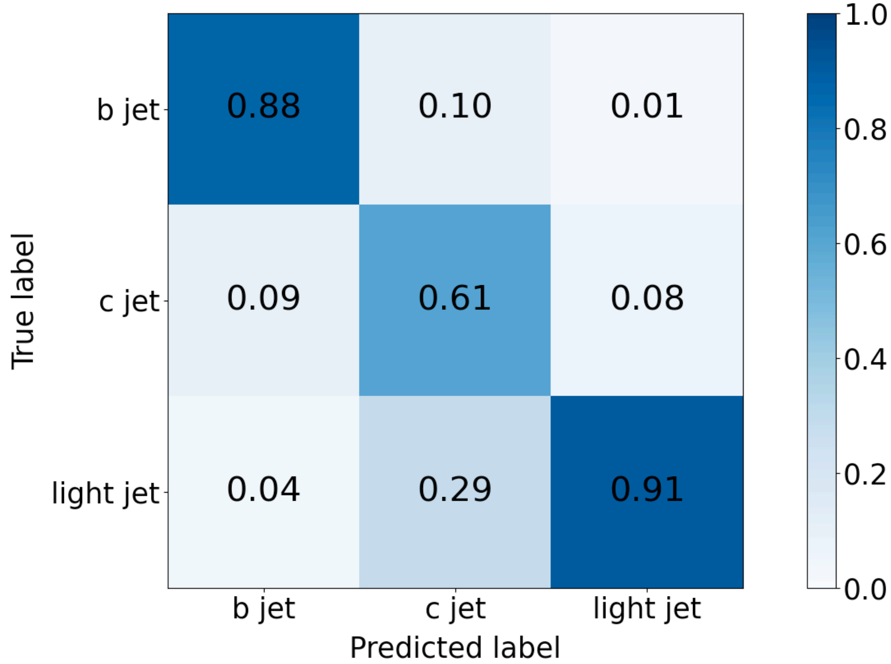
DeepJet: confusion matrices

validation data

efficiency (rows sum up to 1)



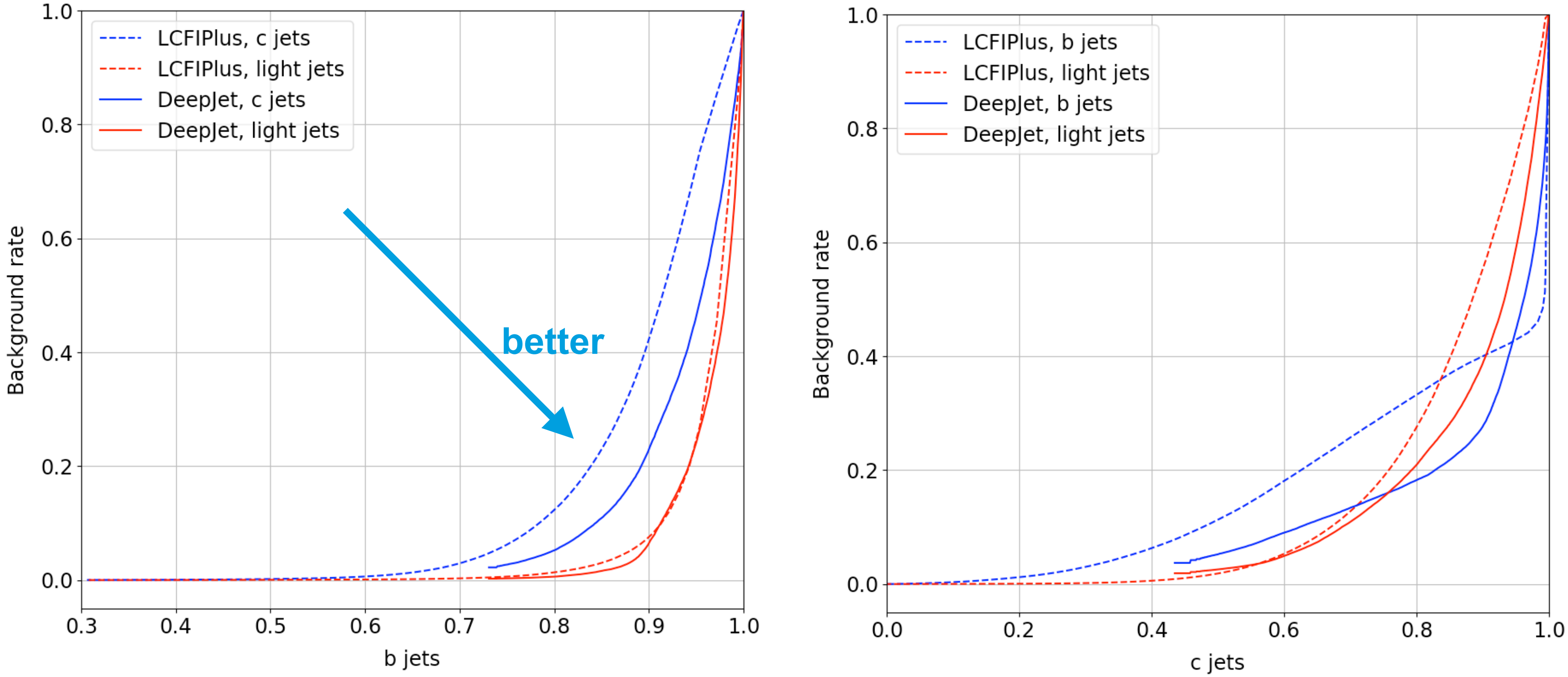
purity (columns sum up to 1)



- identification **efficiencies of over 82% for b jets & light jets**
- **c jet** identification **efficiency** lower (**70%**)
- especially **separation between c jets and light jets should be improved**

DeepJet: ROC curves - comparison to LCFIPlus

validation data



better performance of DeepJet training **over large parts of the b & c tagging efficiencies** w.r.t default LCFIPlus used in ILD

ParticleNet

ParticleNet: input features

jet constituents: coordinates

$\Delta\eta$, $\Delta\Phi$

jet constituents: features

$\Delta\eta$, $\Delta\Phi$

$\log(p_T)$, $\log(E)$, $\log(p_T/p_T^{jet})$, $\log(E/E^{jet})$, $\vec{p}^{\,track} \cdot \vec{p}^{\,jet}/p^{jet}$

ΔR

q

isElectron, isMuon, isChargedHadron, isNeutralHadron, isPhoton

impact parameter & significances

track used in PV?

lepton related variables

pid variables

$E_{HCAL}/E_{HCAL+ECAL}$

$\chi 2/ndf$

28 input features

secondary vertices: coordinates

$\Delta\eta$, $\Delta\Phi$

secondary vertices: features

$\Delta\eta$, $\Delta\Phi$

$\log(p_T)$, E_{SV}/E_{jet}, E_{SV}

η

m_{SV}

$N_{tracks\ in\ SV}$

$\chi 2/ndf$

impact parameters &significances

cos(flight direction$_{SV}$, $\vec{p}_{SV}$)

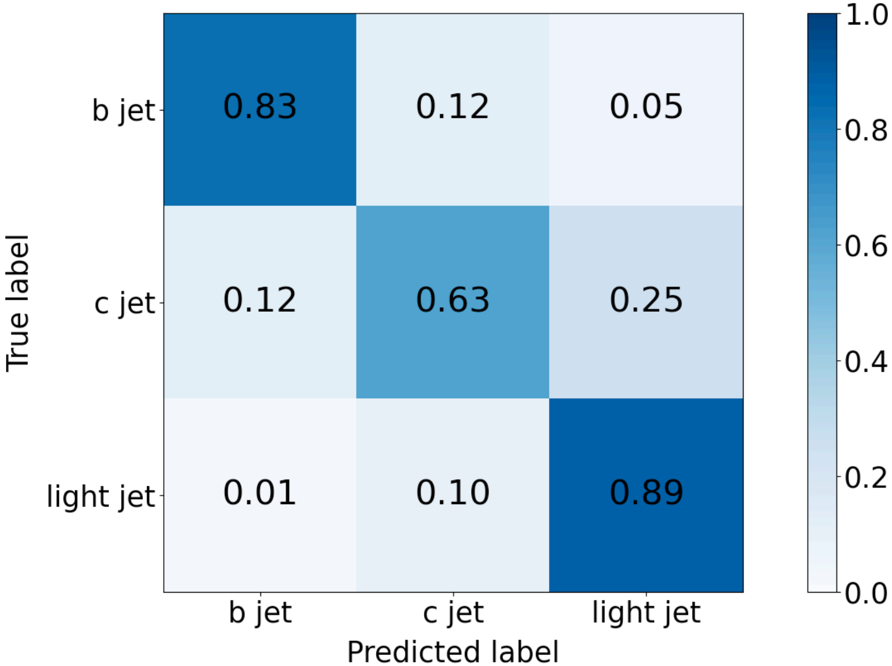
14 input features

2 SVs & all jet constituents considered, no ordering of inputs

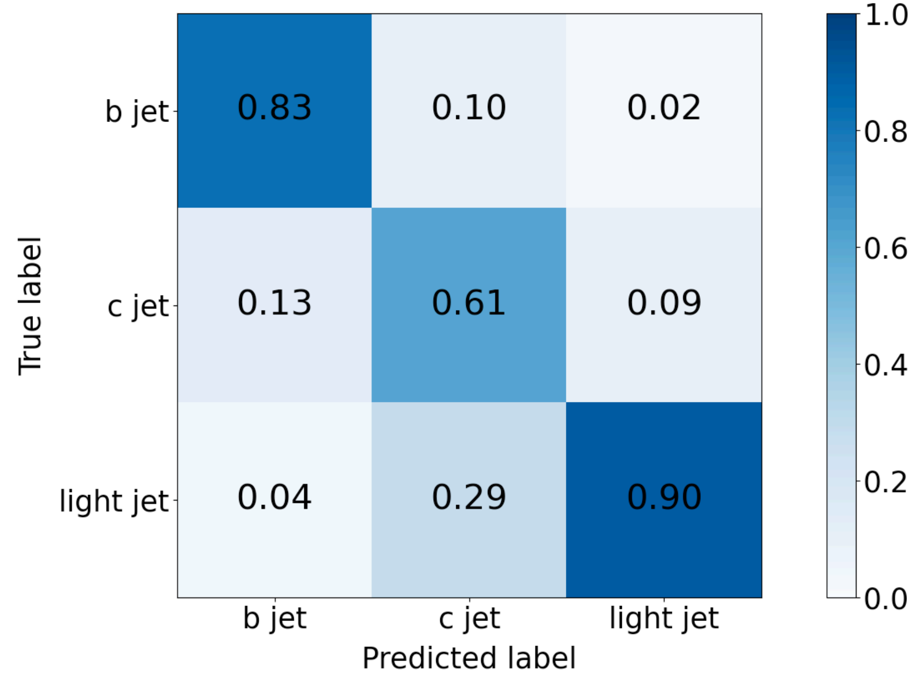
ParticleNet: confusion matrices

validation data

efficiency (rows sum up to 1)



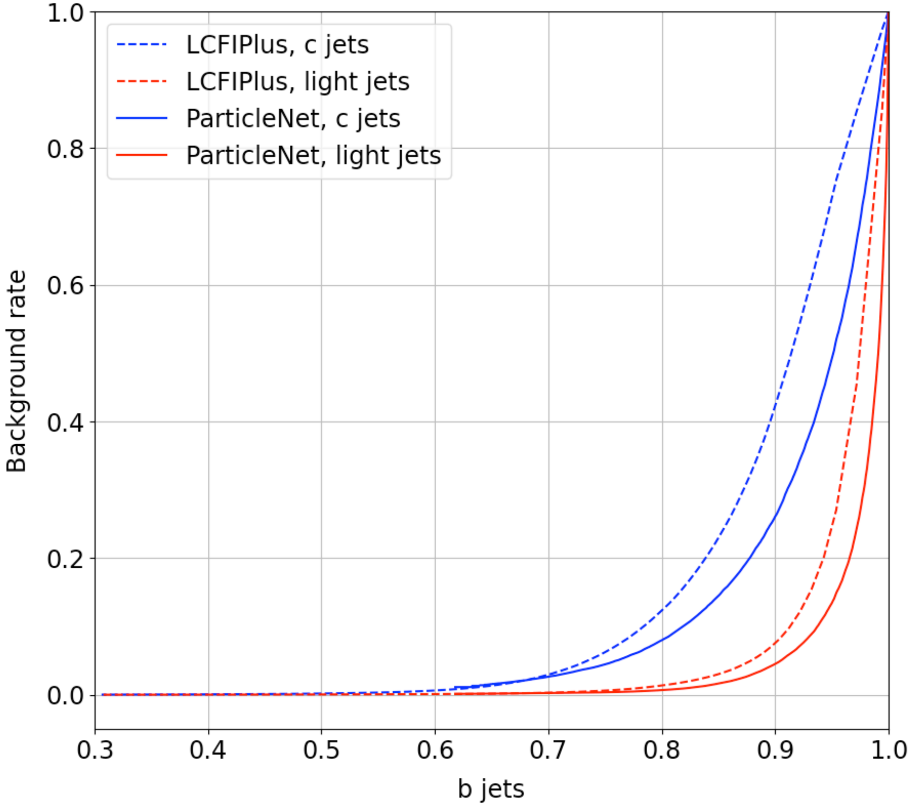
purity (columns sum up to 1)

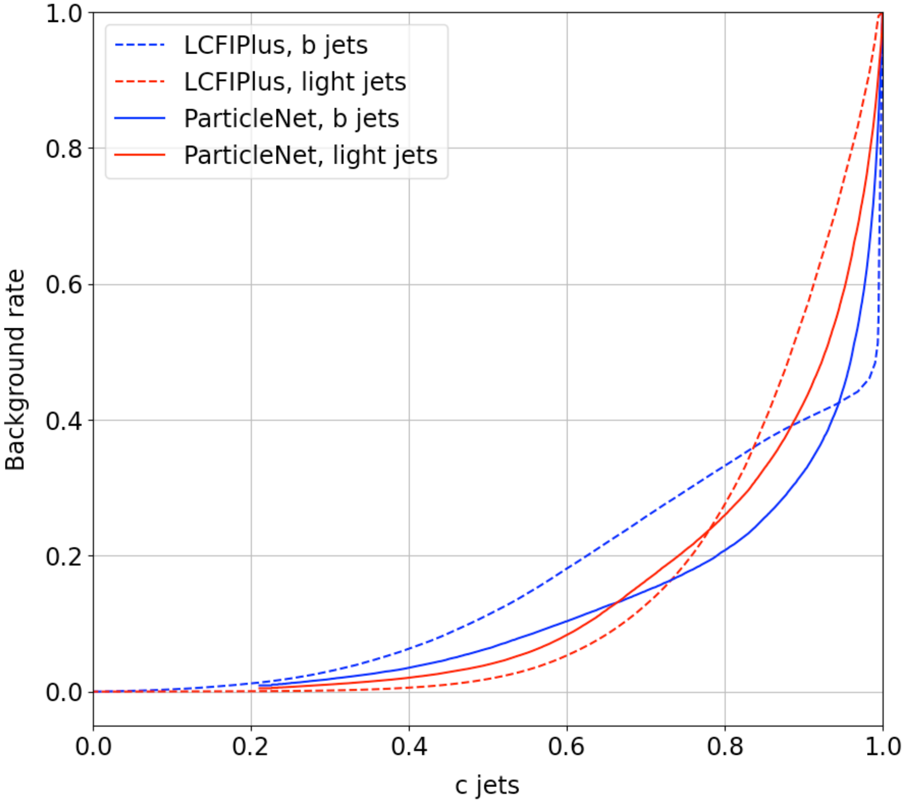


- identification **efficiencies of over 83% for b jets & light jets**
- **c jet** identification **efficiency** quite low (**63%**)
- especially **separation between c jets and light jets should be improved**, larger confusion of c jets with b jets than with DeepJet training

ParticleNet: ROC curves - comparison to LCFIPlus

validation data



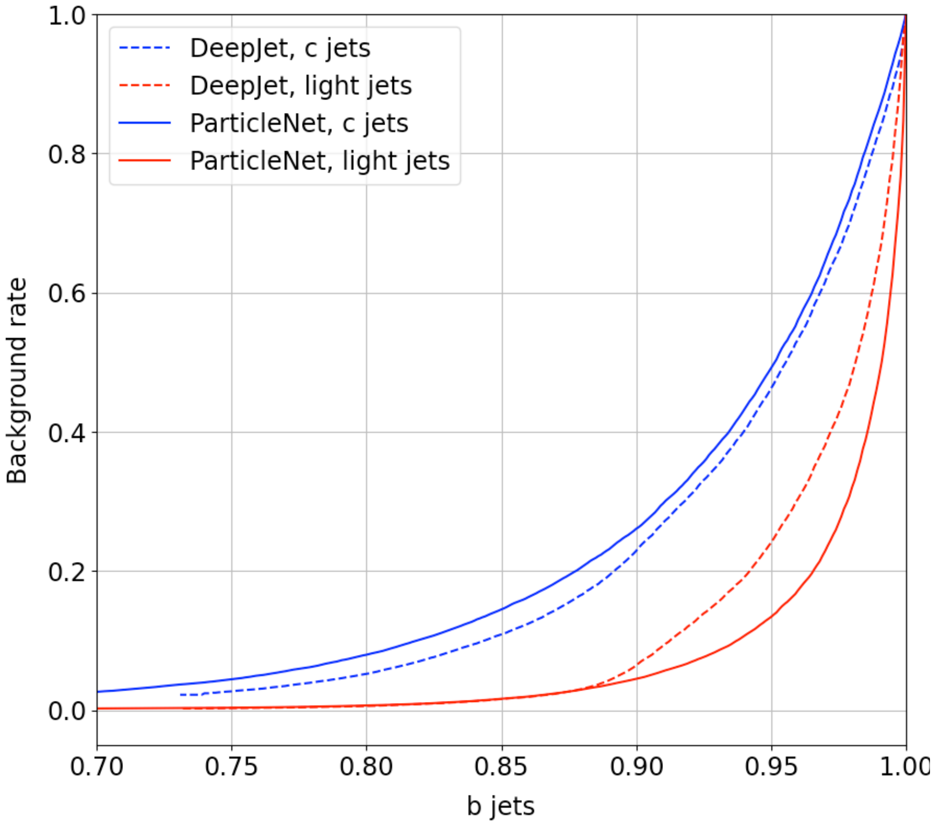


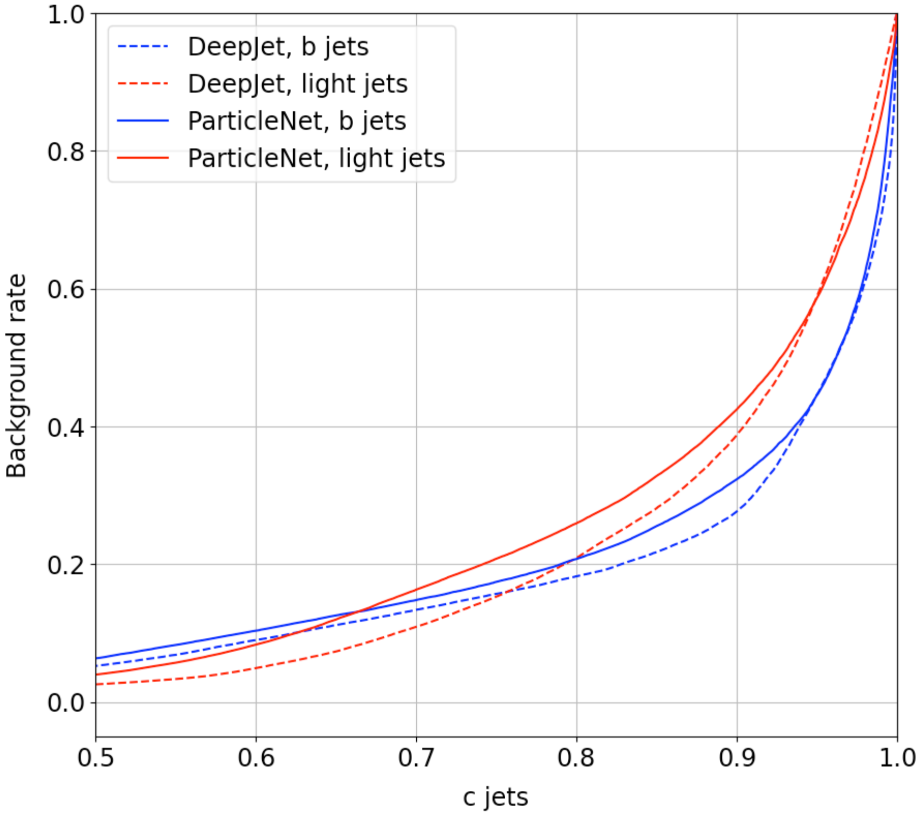
better performance than LCFIPlus **over large parts of the b and c tagging efficiencies**

one of the first trainings with this architecture, **a lot of possibilities for optimization** (architecture, hyperparameters, features, over-training in c-jet category…)

ParticleNet: ROC curves - comparison to DeepJet

validation data





better performance with **DeepJet** for **b vs. c identification and for c vs. b & light jet identification**

better performance of **ParticleNet** for **b jet vs. light jet identification**

Summary & outlook

- application of **CMS DeepJet** tagger and **ParticleNet to ILD**
- **(large) improvements** in **b and c jet identification vs. c/b and light jet background** w.r.t. default LCFIPlus used in ILD
- **ParticleNet** model **not yet optimized**
  - ➡ a lot of possibilities to further improve performance

Outlook:

- **further optimization** of ParticleNet model
- study **performance** on **different processes**
- study **s-tagging efficiency**
- integrate into **iLCSoft/Key4hep** to make the taggers usable for others

Thank you for your attention!

Backup

Training data: details

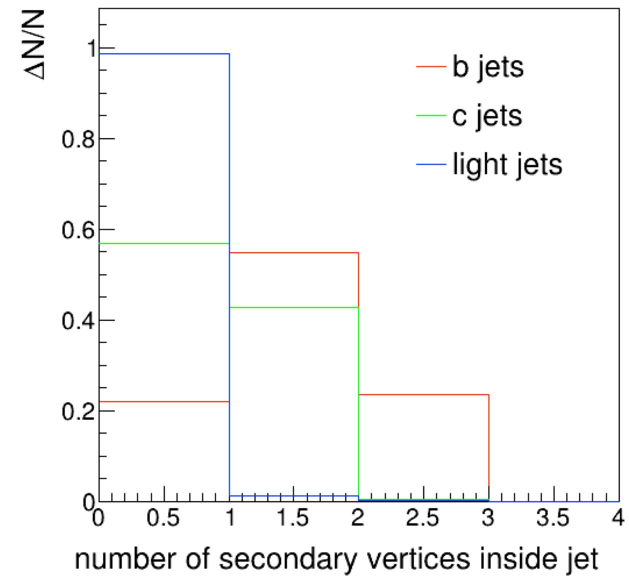
- study **events with 6 jets** (b,c,u,d,s)
  - /pnfs/desy.de/ilc/prod/ilc/mc-opt-3/ild/dst-merged/500-TDR_ws/flavortag/ILD_l5_o1_v02/v02-00-01/
- run PV & SV finder, jet clustering and vertex refinement of LCFIPlus

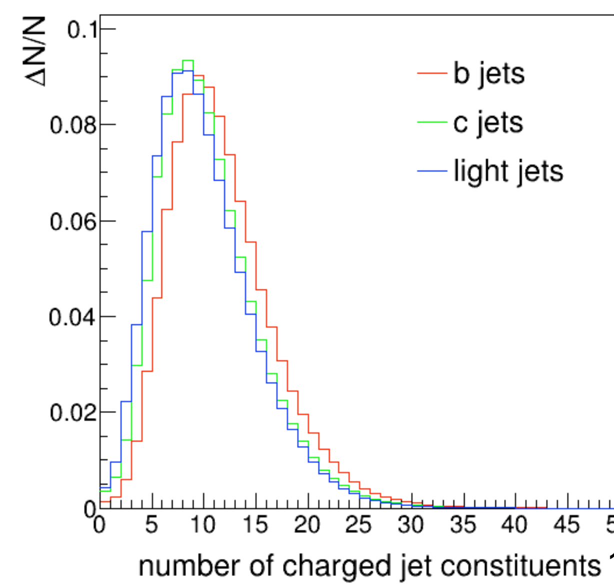
- split sample into training, validation and test (75% / 12.5% / 12.5%)
- number of jets in **training data**:
  - b jets: 434116
  - c jets: 484034
  - light jets: 1449546
  - ➡ over-sampling of b and c jets performed to get same number of b,c & light jets
  - ➡ **total number of jets in training data**: 3 * 1449546 = 4348638
- number of jets in **validation data**:
  - b jets: 72443
  - c jets: 80890
  - light jets: 241283

DeepJet: input features - global variables

21 input features

- jet momentum
- jet transverse momentum
- number of charged jet constituents
- number of neutral jet constituents
- number of secondary vertices
- additional variables from LCFIPlus:
  - mass of all tracks with d0/z0 significance > 5σ
  - product of b/c/light-quark probabilities of d0/z0 values of all tracks, using b/c/light-quark d0/z0 distributions
  - joint probability in the r-φ plane / in the z projection using all tracks (with IP significance > 5σ)
  - vertex probability taking into account all tracks associated to vertex
  - distance and its significance between the first and second vertex in the jet
  - mass of the vertex (pT - corrected)
  - vertex probability of all vertices

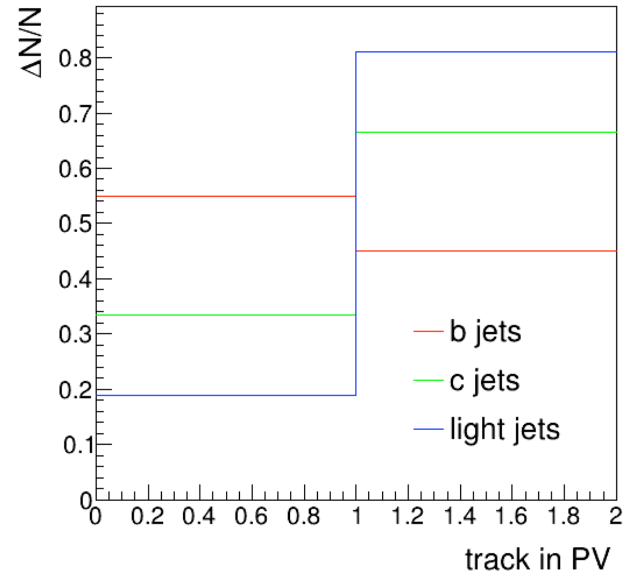


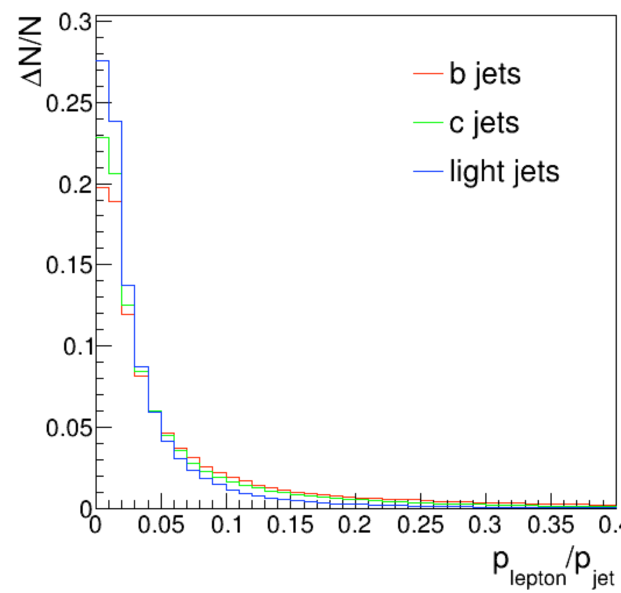


DeepJet: input features - charged jet constituents

- track momentum / jet momentum
- transverse track momentum relative to jet
- dot product of jet and track momentum w.r.t. jet momentum
- ΔR(track, jet),
- d0, d0 significance
- Z0, Z0 significance
- 3D impact parameter, 3D impact parameter significance
- track reconstructed in PV?
- is electron?, is muon?, lepton momentum relative to jet, lepton transverse momentum relative to the jet, lepton momentum / jet momentum
- kaon-ness of charged particles, track momentum fraction weighted with kaon-ness
- χ2/ndf

19 input features

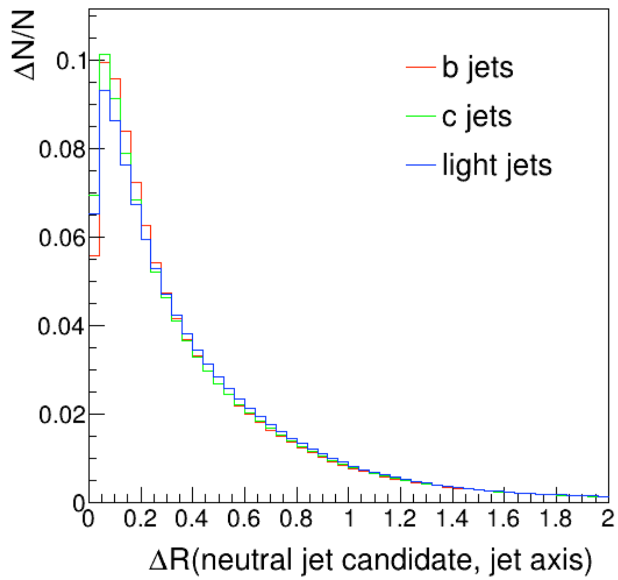


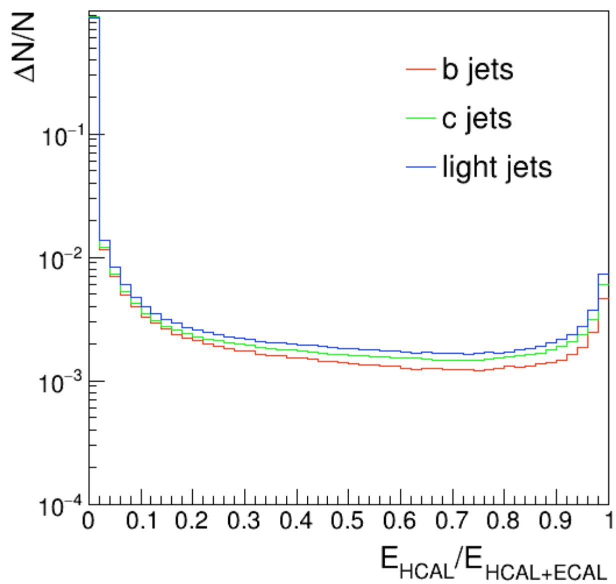


DeepJet: input features - neutral jet constituents

- momentum of neutral jet constituent
- fraction of the jet momentum carried by neutral jet constituent
- ΔR(jet axis, neutral candidate),
- is photon?
- fraction of neutral candidate energy deposited in the hadronic calorimeter

5 input features

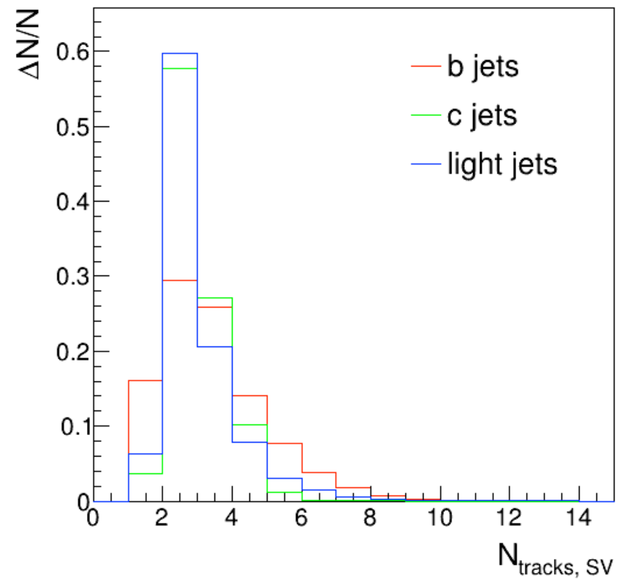


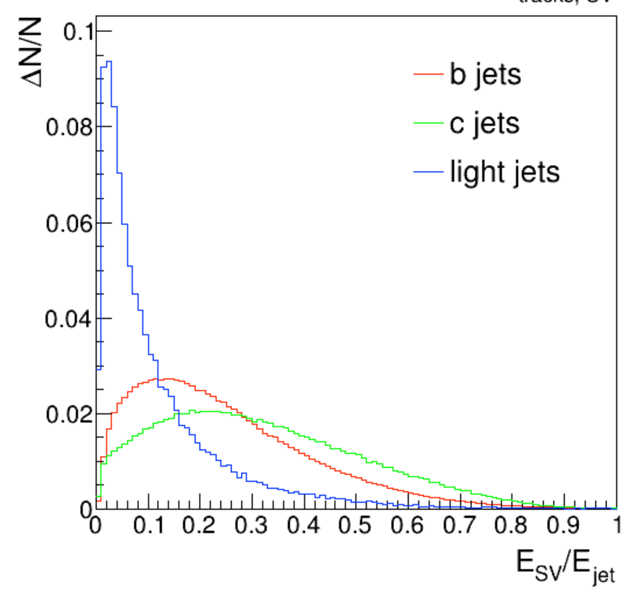


DeepJet: input features - secondary vertices

- SV mass
- number of tracks in SV
- ΔR(SV, jet)
- SV energy / jet energy
- SV energy
- cosine of the angle between the secondary vertex flight direction and the direction of the secodary vertex momentum
- 3D impact parameter, 3D impact parameter significance
- χ2, ndf

10 input features

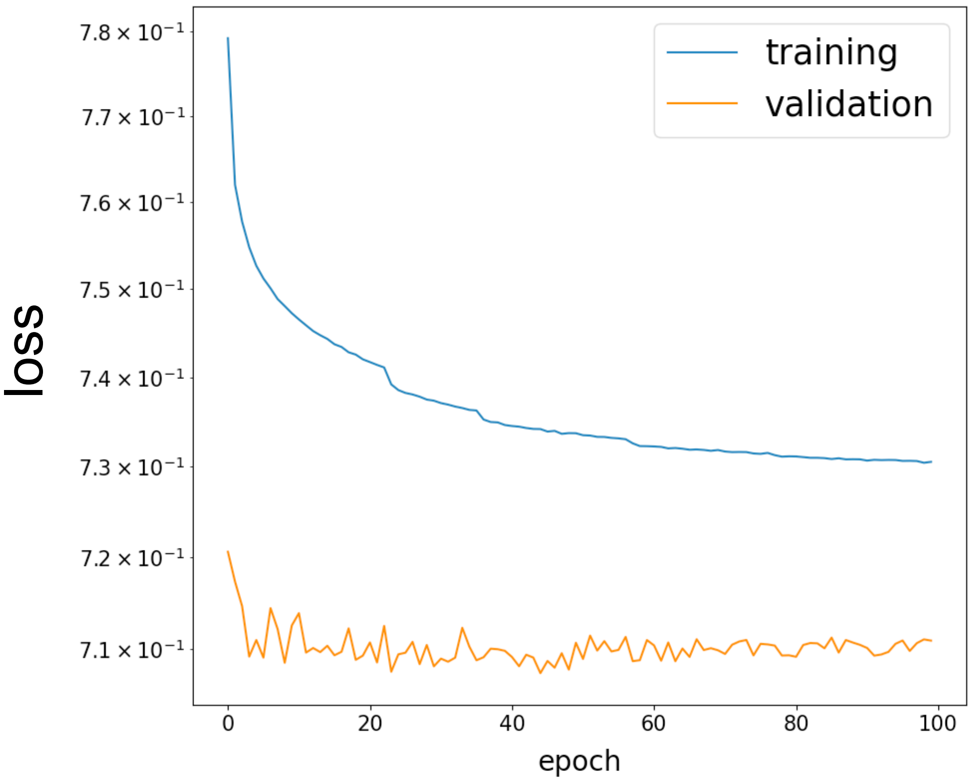


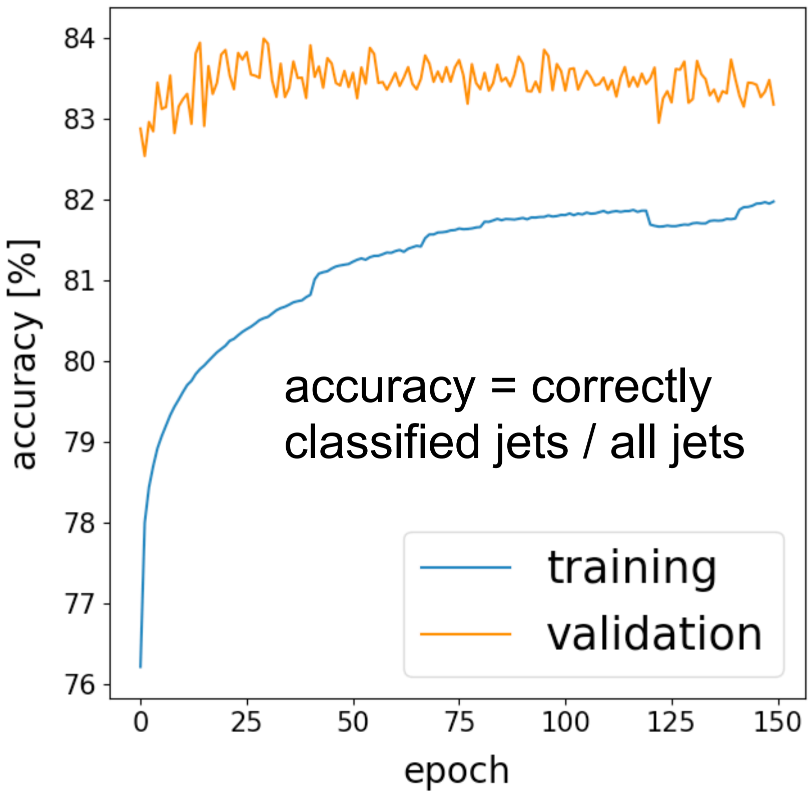


DeepJet: training

- activation functions: relu / softmax (last layer)
- cross entropy loss
- optimizer: Adam
- regularization: batch normalization, dropout (0.1)
- batch size: 200
- learning rate: 0.0003
- number of epochs: 100
- Xavier weight initialization

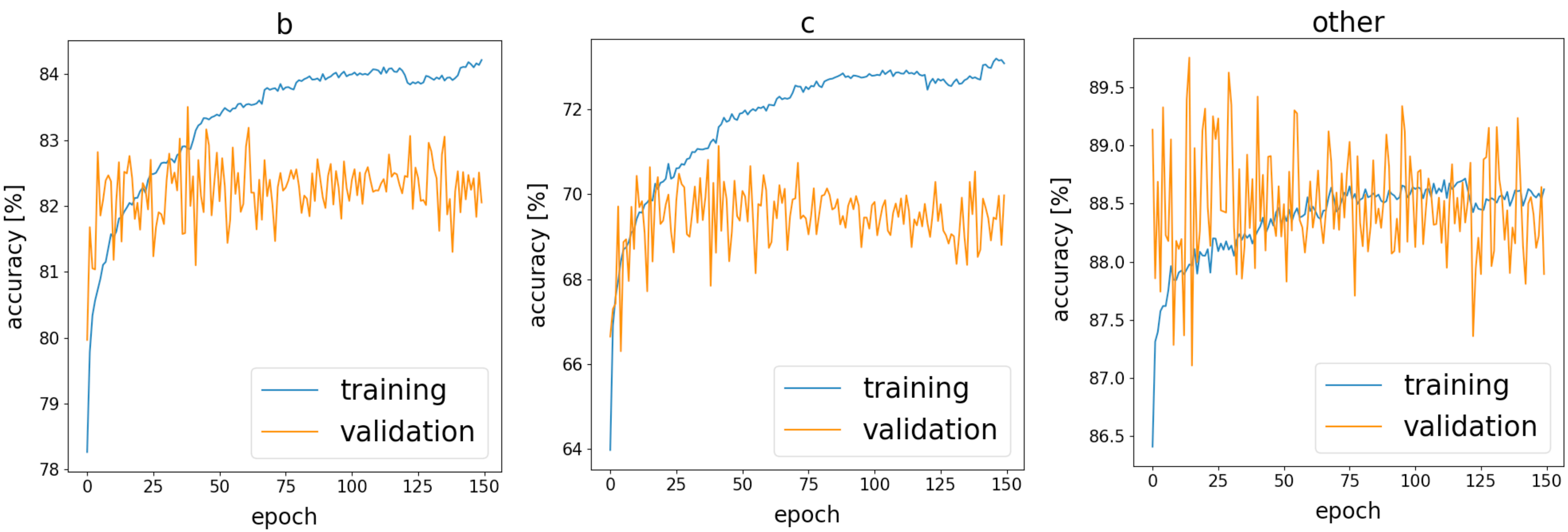
DeepJet: loss & accuracy



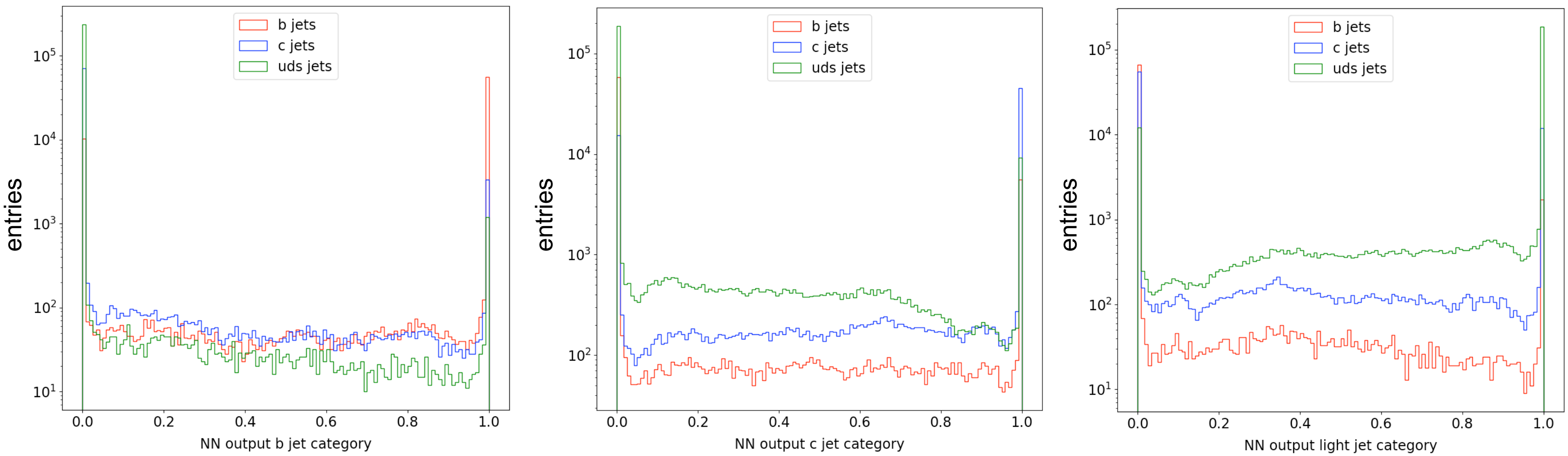


DeepJet: loss & accuracy

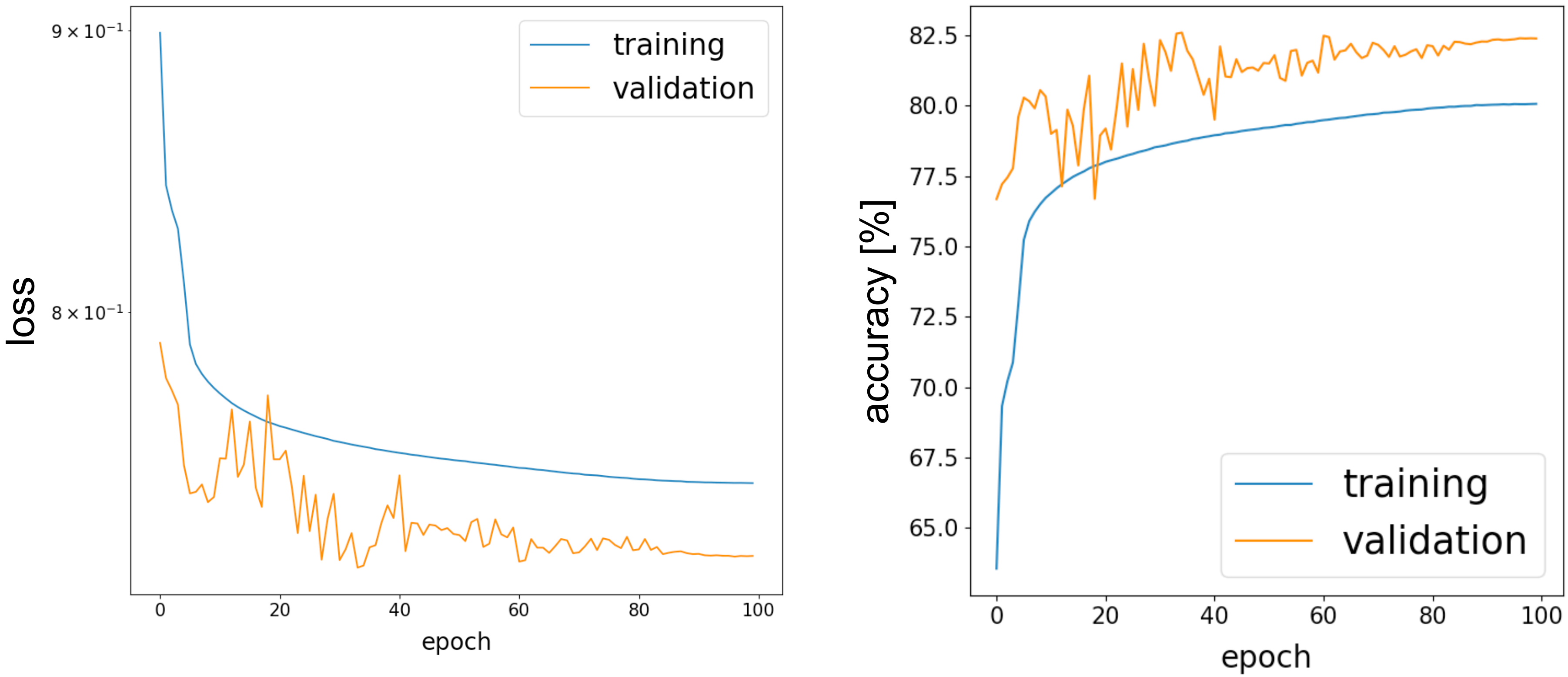
accuracy = correctly classified jets / all jets



DeepJet: NN output

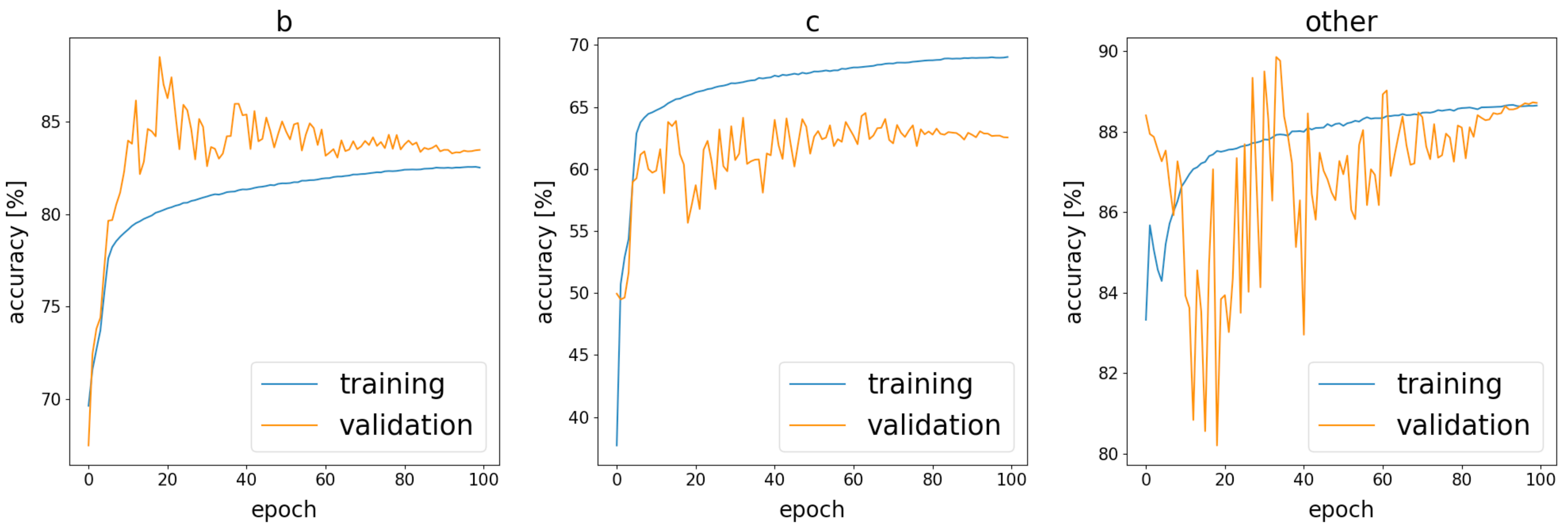


ParticleNet: loss & accuracy

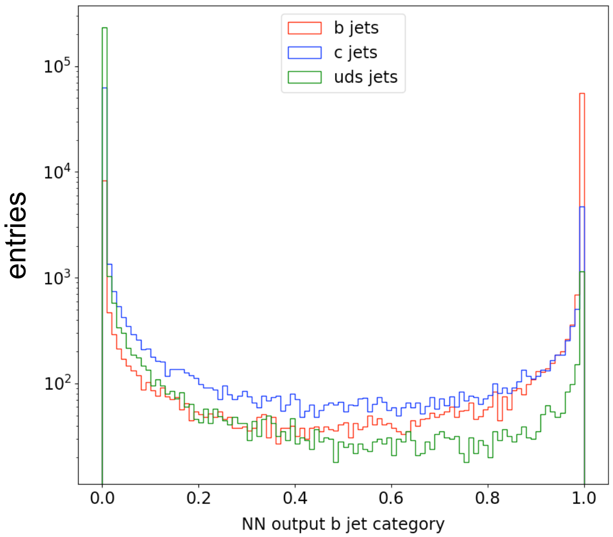


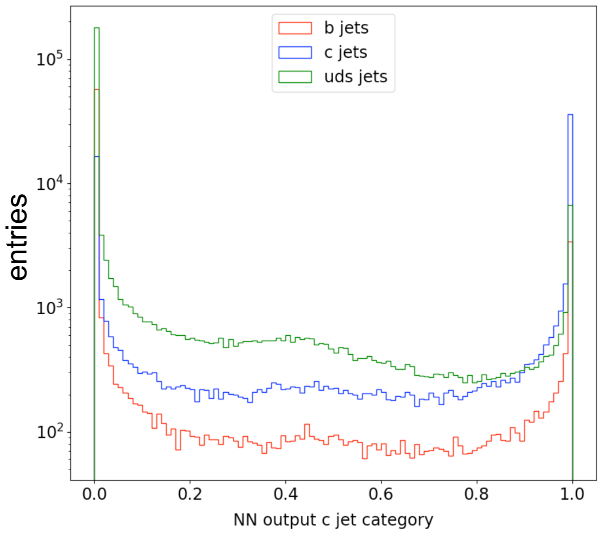
ParticleNet: accuracies

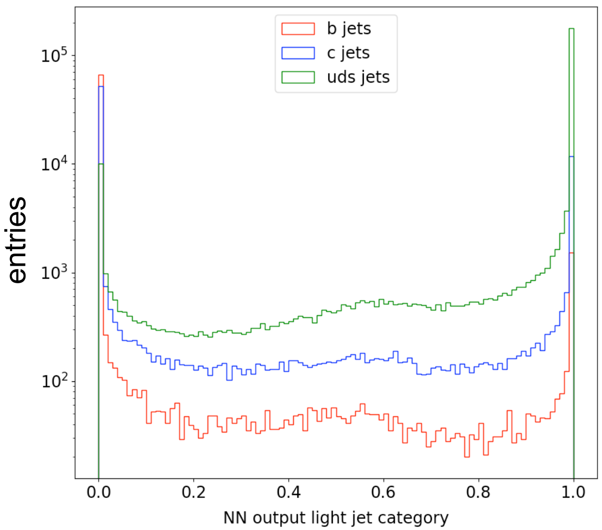
accuracy = correctly classified jets / all jets



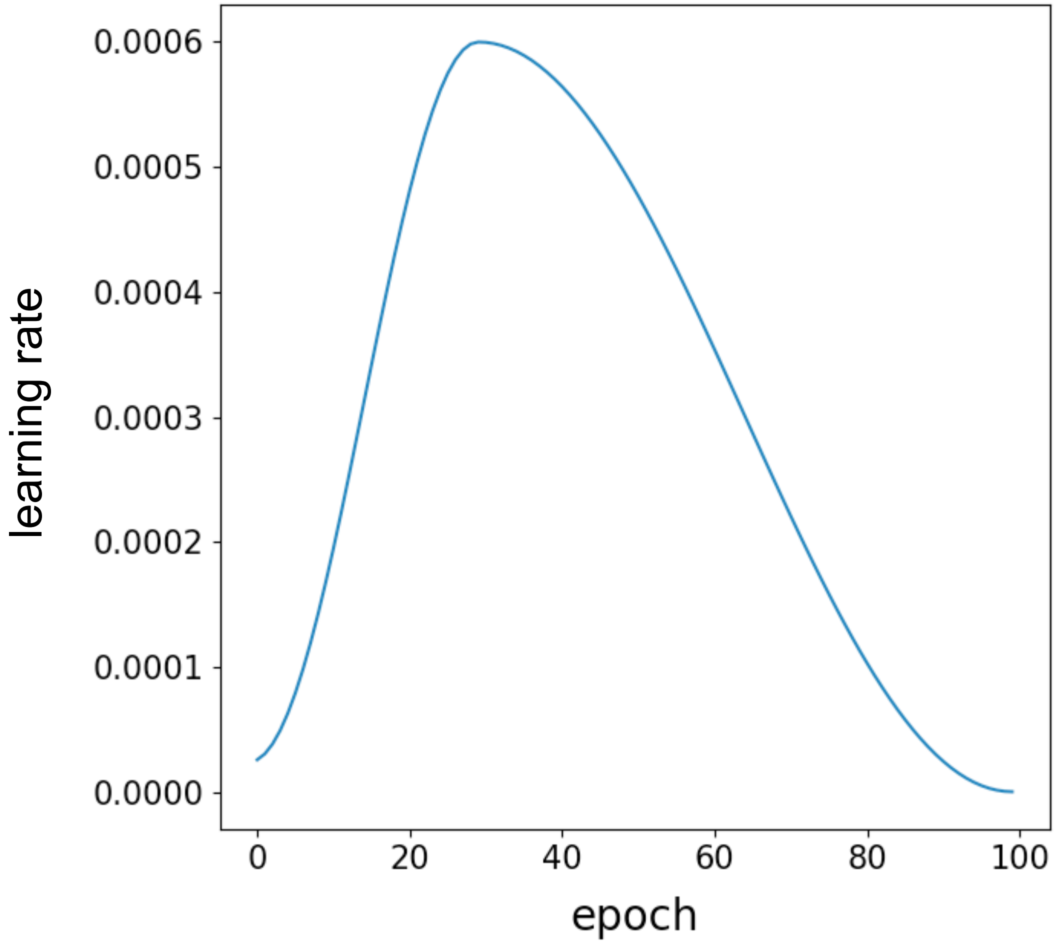
ParticleNet: NN output



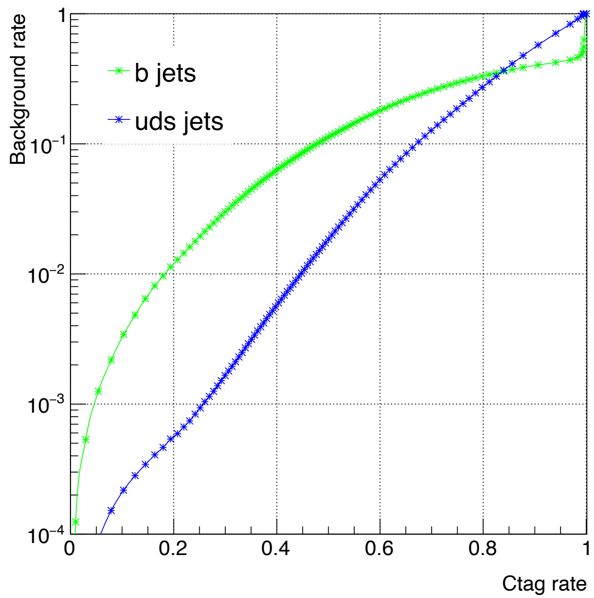


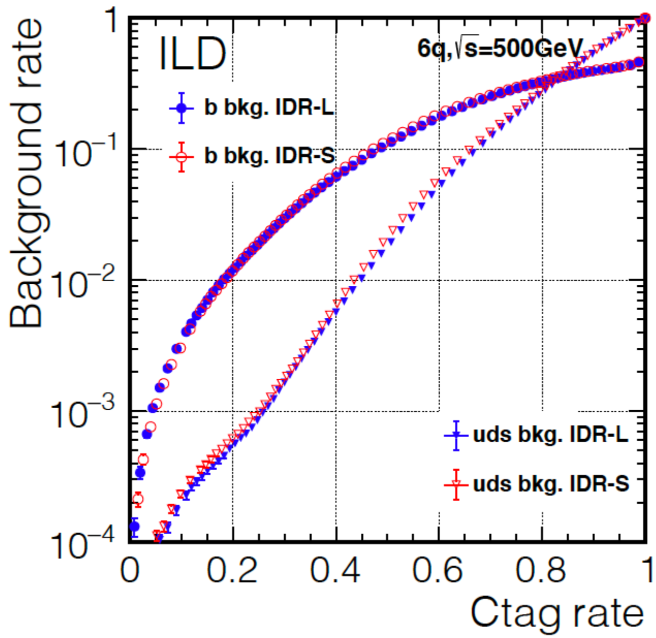


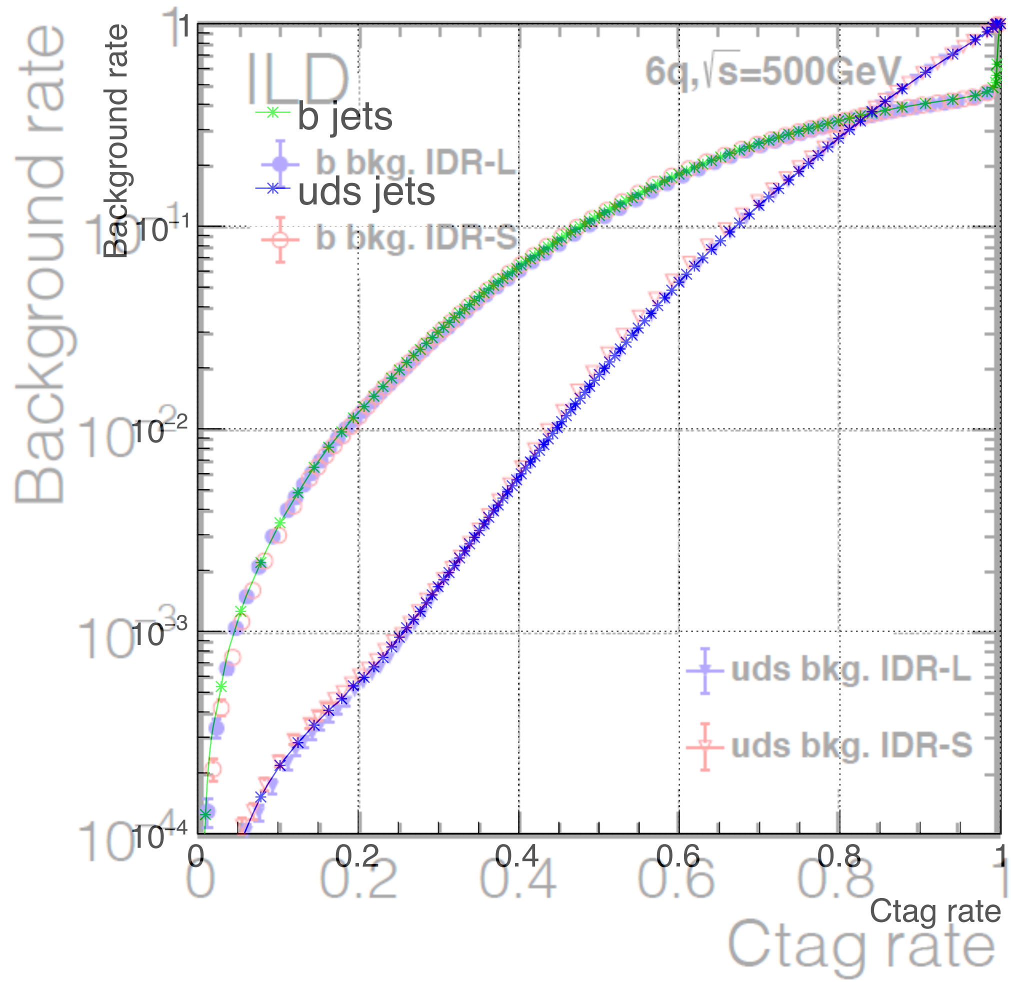
ParticleNet: learning rate



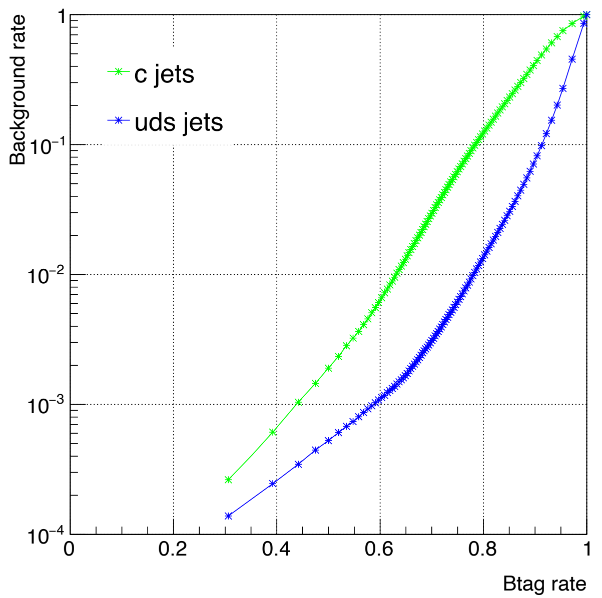
Performance LCFIPlus

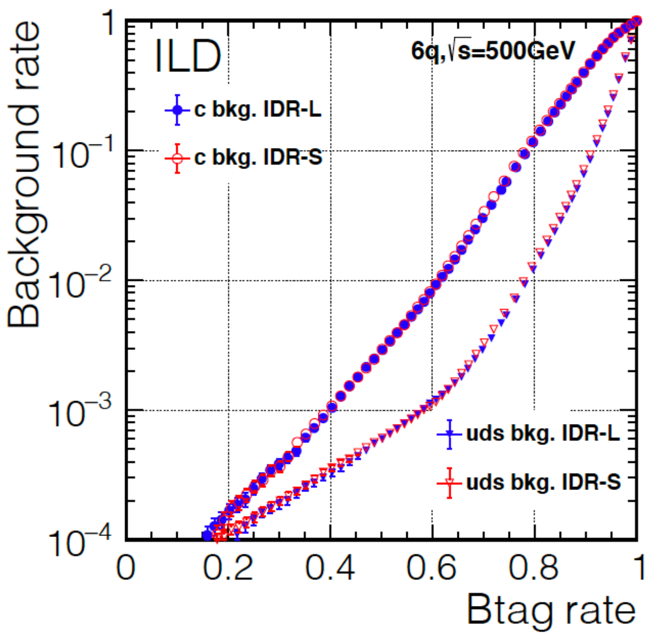


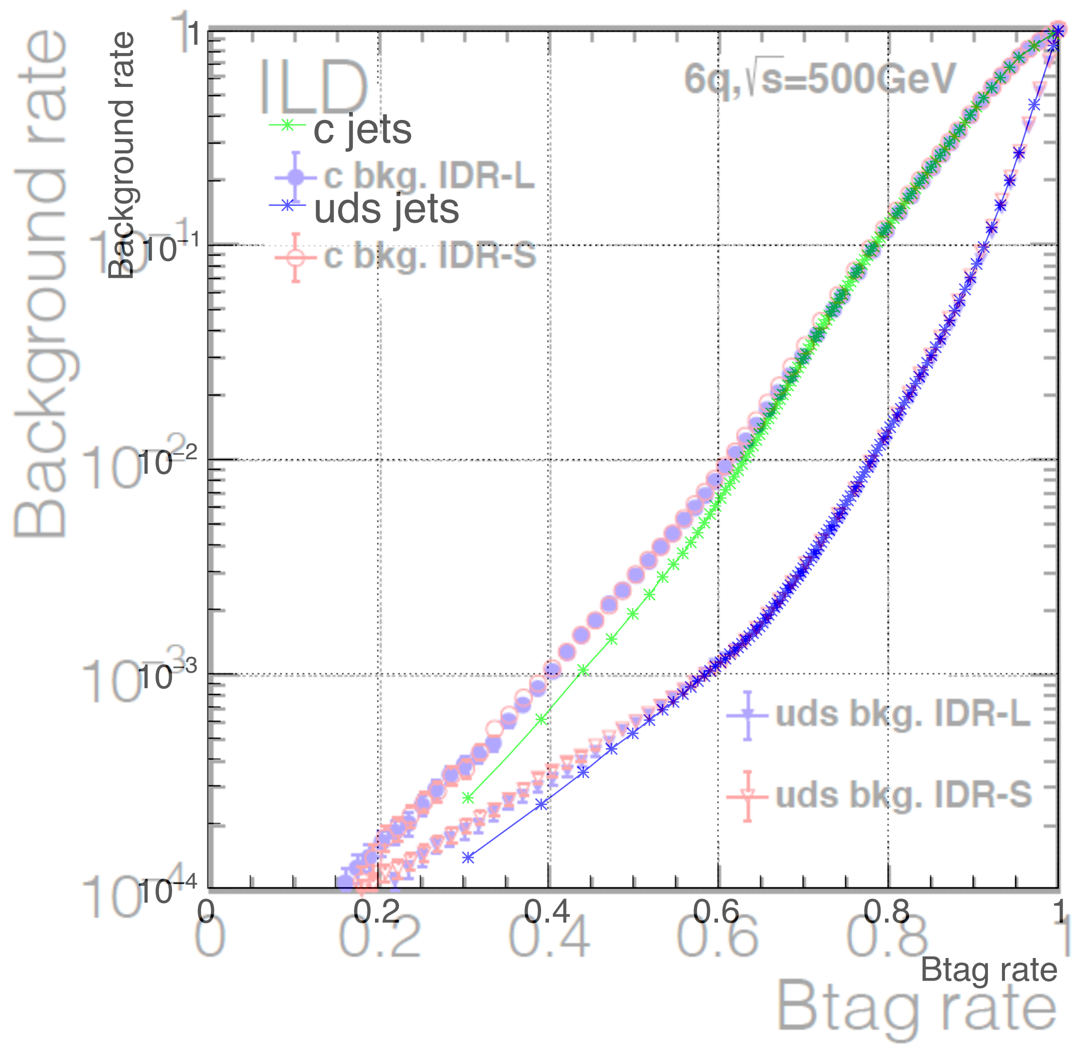




Performance LCFIPlus





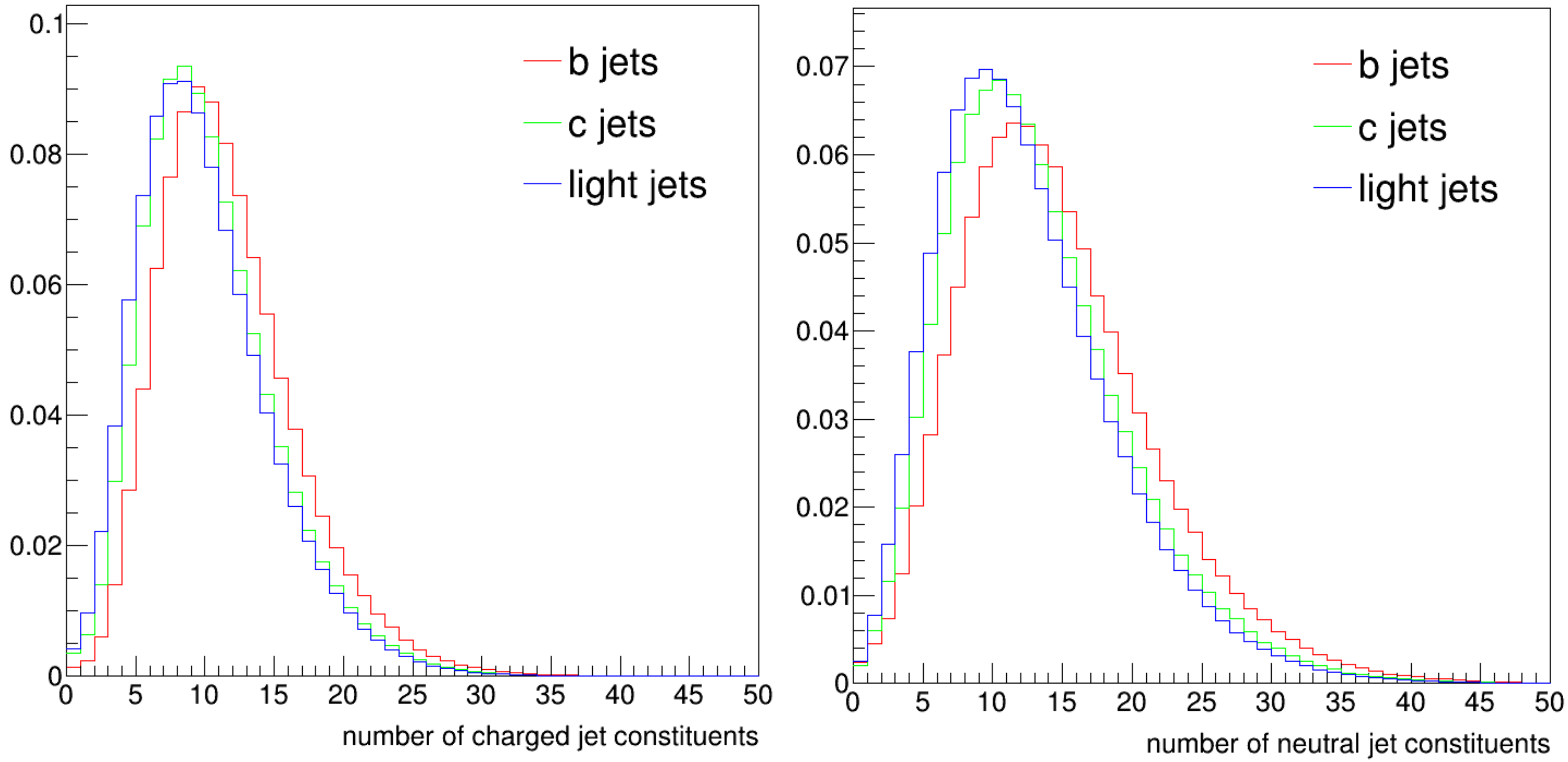


Variables used by LCFIPlus

Name	Description	Normalization factor	Used by category
trk1d0sig	d0 significance of track with highest d0 significance	1	A, B, C, D
trk2d0sig	d0 significance of track with second highest d0 significance	1	A, B, C, D
trk1z0sig	z0 significance of track with highest d0 significance	1	A, B, C, D
trk2z0sig	z0 significance of track with second highest d0 significance	1	A, B, C, D
trk1pt	transverse momentum of track with highest d0 significance	$1/E_{\text{jet}}$	A, B, C, D
trk2pt	transverse momentum of track with second highest d0 significance	$1/E_{\text{jet}}$	A, B, C, D
jprobr	joint probability in the r-phi plane using all tracks	1	A, B, C, D
jprobr5sigma	joint probability in the r-phi plane using all tracks having impact parameter significance exceeding 5 sigma	1	A, B, C, D
jprobz	joint probability in the z projection using all tracks	1	A, B, C, D
jprobz5sigma	joint probability in the z projection using all tracks having impact parameter significance exceeding 5 sigma	1	A, B, C, D
d0bprob	product of b-quark probabilities of d0 values for all tracks, using b/c/q d0 distributions	1	A, B, C, D
d0cprob	product of c-quark probabilities of d0 values for all tracks, using b/c/q d0 distributions	1	A, B, C, D
d0qprob	product of q-quark probabilities of d0 values for all tracks, using b/c/q d0 distributions	1	A, B, C, D
z0bprob	product of b-quark probabilities of z0 values for all tracks, using b/c/q z0 distributions	1	A, B, C, D
z0cprob	product of c-quark probabilities of z0 values for all tracks, using b/c/q z0 distributions	1	A, B, C, D
z0qprob	product of q-quark probabilities of z0 values for all tracks, using b/c/q z0 distributions	1	A, B, C, D
nmuon	number of identified muons	1	A, B, C, D
nelectron	number of identified electrons	1	A, B, C, D
trkmass	mass of all tracks exceeding 5 sigma significance in d0/z0 values	1	A, B, C, D

Variables used by LCFIPlus

Name	Description	Normalization factor	Used by category
1vtxprob	vertex probability with all tracks associated in vertices combined	1	B, C, D
vtxlen1	decay length of the first vertex in the jet (zero if no vertex is found)	$1/E_{\mathrm{jet}}$	B, C, D
vtxlen2	decay length of the second vertex in the jet (zero if number of vertex is less than two)	$1/E_{\mathrm{jet}}$	D
vtxlen12	distance between the first and second vertex (zero if number of vertex is less than two)	$1/E_{\mathrm{jet}}$	D
vtxsig1	decay length significance of the first vertex in the jet (zero if no vertex is found)	$1/E_{\mathrm{jet}}$	B, C, D
vtxsig2	decay length significance of the second vertex in the jet (zero if number of vertex is less than two)	$1/E_{\mathrm{jet}}$	D
vtxsig12	vtxlen12 divided by its error as computed from the sum of the covariance matrix of the first and second vertices, projected along the line connecting the two vertices	$1/E_{\mathrm{jet}}$	D
vtxdirang1	the angle between the momentum (computed as a vector sum of track momenta) and the displacement of the first vertex	E_{jet}	B, C, D
vtxdirang2	the angle between the momentum (computed as a vector sum of track momenta) and the displacement of the second vertex	E_{jet}	D
vtxmult1	number of tracks included in the first vertex (zero if no vertex is found)	1	B, C, D
vtxmult2	number of tracks included in the second vertex (zero if number of vertex is less than two)	1	D
vtxmult	number of tracks which are used to form secondary vertices (summed for all vertices)	1	D
vtxmom1	magnitude of the vector sum of the momenta of all tracks combined into the first vertex	$1/E_{\mathrm{jet}}$	B, C, D
vtxmom2	magnitude of the vector sum of the momenta of all tracks combined into the second vertex	$1/E_{\mathrm{jet}}$	D
vtxmass1	mass of the first vertex computed from the sum of track four-momenta	1	B, C, D
vtxmass2	mass of the second vertex computed from the sum of track four-momenta	1	D
vtxmass	vertex mass as computed from the sum of four momenta of all tracks forming secondary vertices	1	B, C, D
vtxmasspc	mass of the vertex with minimum pt correction allowed by the error matrices of the primary and secondary vertices	1	B, C, D
vtxprob	vertex probability; for multiple vertices, the probability P is computed as 1-P = (1-P1)(1-P2)...(1-PN)	1	B, C, D


0.1
0.08
0.06
0.04
0.02
0
0
5
10
15
20
25
30
35
40
45
50
b jets
c jets
light jets
number of charged jet constituents
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
5
10
15
20
25
30
35
40
45
50
b jets
c jets
light jets
number of neutral jet constituents